(Quantum) Chaos in BECs

S.A. Gardiner

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The achievement of Bose-Einstein condensation of a dilute vapour of Rubidium atoms in 1995 [1] heralded the beginning of a rapidly growing field of experimental and theoretical endeavour, each of which has further stimulated the other. In the intervening years, the experimental production of Bose-Einstein condensates (BECs), particularly of Rubidium and Sodium vapours, has become almost routine, and attention has shifted to either the condensation of more exotic species (of particluar note is the recent successful condensation of metastable helium [2]); or to deeper experimental investigations of the properties of an atomic BEC, up to the point of viewing a BEC more as a tool rather than an end in itself. The purpose here is to show links between chaotic dynamics, both in a classical and a quantum mechanical sense, and the possibly "chaotic" dynamical and stability properties of BECs.

To begin: considering only the dynamics of a single *classical* point particle of mass m, one can reasonably speak of a class of "chaos-inducing" potentials $V_c(\mathbf{x})$, such that a particle can exhibit chaotic dynamics under the influence of such a potential. One can qualitatively visualize chaotic dynamics as being highly irregular motion in *phase space*. For a particle moving in one spatial dimension this is a two-dimensional space, where (subject to canonical changes of variables) the axes correspond to the particle's position x and momentum p. Such highly irregular motion is generally associated with *exponential sensitivity to initial conditions*, i.e. small differences in a point particle's initial position and momentum can make a large difference in its long-time behaviour. The appropriate classical (Hamilton's) equations of motion can then be derived from a Hamiltonian function of the general form:

$$H = \frac{\mathbf{p}^2}{2m} + V_c(\mathbf{x}). \tag{1}$$

One can readily make the jump to quantum mechanics by replacing the number-valued position and momentum variables with *operator* quantities. For a single particle, the dynamics are then generally most conveniently described by the following *Schrödinger equation*:

$$i\hbar\frac{\partial\psi(\mathbf{x})}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m} + V_c(\mathbf{x})\right]\psi(\mathbf{x}). \tag{2}$$

This is clearly a *linear* partial differential equation, where the time-derivative of the wavefunction $\psi(\mathbf{x})$ is proportional to the Hamiltonian *operator* [the momenta $\mathbf{p} = (p_x, p_y, p_z)$ have been replaced by differential operators] acting on $\psi(\mathbf{x})$. As chaos

is generally associated with nonlinear differential equations, this can cause some to question how one can speak of quantum chaos at all. In classical mechanics we are interested in the motion of the particle in phase space, and thus in the changes of its position and momentum with time. The classical dynamics of a point particle's position and momentum, and the dynamics of the quantum wavefunction $\psi(\mathbf{x})$ are thus not really directly comparable: better analogies exist between Heisenberg's equations and Hamilton's equations of motion, or alternatively between Schrödinger's equation and Liouville's equation. Here quantum chaos is considered to be the study of quantum dynamical systems, the classical limits of which are capable of exhibiting chaotic dynamics. That Schrödinger's equation is a linear partial differential equation is in this context an irrelevancy; nevertheless it is interesting to consider the effect of introducing an explicit nonlinearity into a quantum-chaotic Schrödinger equation:

$$i\hbar \frac{\partial \psi(\mathbf{x})}{\partial t} = \left[-\frac{\hbar^2 \nabla^2}{2m} + V_c(\mathbf{x}) + u|\psi(\mathbf{x})|^2 \right] \psi(\mathbf{x}). \tag{3}$$

One could regard such an equation as describing "nonlinear quantum chaos" or "nonlinear wave chaos." Such *nonlinear Schrödinger equations* are relevant for nonlinear optics, but more pertinently are extensively used to describe BECs, when they are called *Gross-Pitaevskii* equations [3]. A Gross-Pitaevskii equation is used as an *approximate* description of the dynamics of a large number N of (bosonic) interacting quantum mechanical particles, which is more fully described by a quantum field; if nearly all of these particles can be considered to be in the same motional state $\psi(\mathbf{x})$ (i.e. if we have a BEC), then it is possible to describe most of the underlying quantum field by a classical field, and to regard what is left over as being "small." The Gross-Pitaevskii equation is then the equation of motion of this classical field. It is nevertheless sometimes necessary to consider the dynamics of the full quantum field; in second-quantized form, the Hamiltonian operator leading to such a Gross-Pitaevskii equation (with $u = gN$ and g being a parameter essentially describing how strongly individual particles interact) is given by

$$\hat{H} = \int d^3\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_c(\mathbf{x}) + \frac{g}{2} \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \right] \hat{\psi}(\mathbf{x}), \tag{4}$$

where $\hat{\psi}^\dagger(\mathbf{x})$ and $\hat{\psi}(\mathbf{x})$ are bosonic field *operators*, which create and annihilate, respectively, a particle at position $\mathbf{x}$. In this context, one could thus possibly speak of "quantum field chaos" when considering the dynamics induced by such a Hamiltonian.

A brief discussion of integrability, a concept closely tied to the (non) chaoticity of dynamical systems, is now necessary [4]. Recalling the classical dynamics of a *single* particle, such a system is considered integrable if there exist as many independent conserved quantities as there are motional degrees of freedom (i.e. the number of relevant spatial dimensions). If the system *is* integrable, then the phase-space dynamics of the particle are so restricted by the necessity of observing these conservation laws that chaos is impossible. To take the rather trivial example of the one-dimensional harmonic oscillator [potential $V(x) = m\omega^2 x^2/2$], the solution of Hamilton's equations of motion (in slightly unconventional form) is given by:

$$\alpha(t) = e^{-i\omega t} \alpha(0), \tag{5}$$

where α is a complex variable, defined as

$$\alpha = \frac{m\omega x + ip}{\sqrt{2m}}. \tag{6}$$

It is clear that the particle motion is restricted to closed circles in the two-dimensional phase space, making both "irregular" motion in phase space, and sensitivity to initial conditions completely impossible. In the language of Hamilton-Jacobi theory, $|\alpha(t)|$ is an action variable, which is conserved (and equal to the square root of the energy), and the dynamics are fully described by the time-evolution of the phase angle of $\alpha(t)$, which is then the canonically conjugate angle variable $\theta(t)$ to $|\alpha(t)|$, defined by

$$\theta = \arctan\left(\frac{p}{m\omega x}\right). \tag{7}$$

Similar analyses can be made for any one-dimensional, time independent system; due to the time-independence of the Hamiltonian, the energy is always a conserved quantity, which is enough to make a one-dimensional system integrable. Two- and three-dimensional systems will require additional *independent* conserved quantities to be integrable, and time dependence in a one-dimensional system generally lifts the property of integrability. Concepts of quantum integrability generally, by analogy, consider conserved *observable* quantities, which in quantum mechanics are described by operators [4]; it is possible to consider something different however.

A wavefunction $\psi(\mathbf{x})$ can generally be decomposed in terms of some complete orthonormal basis [5]:

$$\psi(\mathbf{x}) = \sum_{k=0}^{\infty} c_k \varphi_k(\mathbf{x}). \tag{8}$$

If additionally the $\varphi_k(x)$ are eigenfunctions of the (assumed time-independent) Hamiltonian, then any time dependence of $\psi(x)$ is contained completely within the coefficients c_k: thus

$$c_k(t) = e^{-i\omega_k t} c_k(0). \tag{9}$$

For example, in the case of a one-dimensional *quantum* harmonic oscillator, the $\varphi_k(x)$ are Gauss-Hermite polynomials, and $\omega_k = \omega(k + 1/2)$. There is an now an obvious similarity between equations (5) and (9). Extending the analogy, we can consider motion in an infinite-dimensional pseudo phase space of a "point particle" having "position" values

$$\chi_k = c_k + c_k^*, \tag{10}$$

and "momentum" values of

$$\rho_k = -i(c_k - c_k^*). \tag{11}$$

Within this pseudo phase space however, as in the case of the classical harmonic oscillator, motion is severely restricted by the fact that all the $|c_k|$ are conserved [6]. The $|c_k|$ (effectively the "action variables" in the pseudo phase space) in fact form a *complete set* of conserved quantities (i.e. there are as many conserved quantities as degrees of freedom), meaning that, in this sense, the Schrödinger equation is *always* integrable and thus *never* chaotic, a fact which is indeed a direct consequence of the Schrödinger equation's linearity.

For a general Gross-Pitaevskii equation, the additional nonlinear term means that integrability clearly cannot be taken for granted. It is, for example, known that the one dimensional, homogeneous case

$$i\hbar\frac{\partial\psi(x)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + u|\psi(x)|^2\right]\psi(x) \tag{12}$$

is integrable [7], and that the conserved quantities can be determined using inverse scattering techniques. However, even for the seemingly trivial extension of simply adding a harmonic potential (generally more relevant to current experiments), it is unknown whether the resulting Gross-Pitaevskii equation is integrable or not; the application of a δ-kicking potential (as is widely considered in the study of classical and quantum chaos)

$$V_c(x) = K\cos(kx)\sum_{n=-\infty}^{\infty}\delta(t-nT), \tag{13}$$

will produce a Gross-Pitaevskii equation which is unlikely to be integrable [8]. This general lack of integrability therefore raises the possibility of chaotic dynamics in the pseudo phase space, including extreme sensitivity to initial conditions.

In classical machanics, sensitivity to initial conditions is generally gauged by the Lyapunov exponent, so that a positive Lyapunov is considered a strong indicator of chaotic dynamics. The Lyapunov exponent is concerned with the growth with time of the euclidean "distance" d in phase space between two initially close point particles. In one dimension, d is thus given by

$$d(t) = \sqrt{[x_1(t)-x_2(t)]^2 + [p_1(t)-p_2(t)]^2}. \tag{14}$$

In the pseudo phase space produced by some orthonormal representation of two initial wavefunctions $\psi_1(x)$ and $\psi_2(x)$, the equivalent d is given by

$$\begin{aligned} d(t) &= \sqrt{\sum_k[\chi_{k1}(t)-\chi_{k2}(t)]^2 + [\rho_{k1}(t)-\rho_{k2}(t)]^2} \\ &= \sqrt{2-\int d^3\mathbf{x}\,[\psi_1^*(\mathbf{x},t)\psi_2(\mathbf{x},t)+\psi_2^*(\mathbf{x},t)\psi_1(\mathbf{x},t)]}, \end{aligned} \tag{15}$$

where in the case of the linear Schrödinger equation, by unitarity $\int d^3\mathbf{x}\psi_1^*(\mathbf{x})\psi_2(\mathbf{x})$ cannot change, and d will therefore be constant [9]. Upon the addition of a nonlinearity this is of course no longer guaranteed, which in the case of the Gross-Pitaevskii equation can have important consequences for the stability of the condensate, due to a correspondance between the propagation of linearized perturbations around the condensate wavefuntion, and propagation (and growth) of the non-condensate fraction.

It is now necessary to return briefly to a fuller quantum mechanical description of the BEC. If the number of particles in the condensate mode is nearly N, the field operator $\hat{\psi}(\mathbf{x})$ can be written as [10, 11]

$$\hat{\psi}(\mathbf{x}) \approx \hat{a}\left[\psi(\mathbf{x}) + \frac{1}{\sqrt{N}}\sum_k \hat{b}_k u_k(\mathbf{x}) + \hat{b}_k^\dagger v_k^*(\mathbf{x})\right]. \tag{16}$$

The $\hat{a}$ operator annihilates a particle in the condensate mode $\psi(\mathbf{x})$ (it is approximately this mode which is propagated by the Gross-Pitaevskii equation if the number of particles in the condensate mode $\hat{a}^\dagger\hat{a} \approx N$), and the $\hat{b}_k^\dagger$ and $\hat{b}_k$ are creation and annihilation operators of *excitations* above the condensate, the $u_k(\mathbf{x})$ and $v_k^*(\mathbf{x})$ describing the spatial dependence of these excitations. These excitation modes clearly describe *non-condensate* particles, and for the idealized case of zero temperature, the number of non-condensate particles is then given by

$$\sum_k \int d^3\mathbf{x}|v_k(\mathbf{x},t)|^2. \tag{17}$$

The excitation modes are propagated by slightly modified Bogoliubov equations, which are identical to the equations derived by considering perturbations around and *orthogonal* to $\psi(\mathbf{x})$ propagated by the Gross-Pitaevskii equation up to *linear* order in the perturbation only. If one then considers

$$\psi_1(\mathbf{x},0) = \psi(\mathbf{x},0), \tag{18}$$

and

$$\psi_2(\mathbf{x},0) = \psi(\mathbf{x},0) + \frac{1}{\sqrt{N}}[u_k(\mathbf{x},0) + v_k^*(\mathbf{x},0)], \tag{19}$$

it is clear that a reduction with time of $|\int d^3\mathbf{x}\psi_1^*(\mathbf{x},t)\psi_2(\mathbf{x},t)|$ directly implies growth in the number of non-condensate particles, and, more generally, growth in the number of non-condensate particles is implied by any kind of linear instability in a solution of the Gross-Pitaevskii equation. Chaotic dynamics in the pseudo phase space thus imply the rapid increase in number of non-condensate particles, which in turn implies rapid depletion of the condensate. There is a caveat to this: the derivation of the equations used in the analysis formally take the limit $N \to \infty$, $g \to 0$, while keeping gN constant. There is therefore *formally* an infinite number of condensate particles, which stays infinite as the number of non-condensate particles increases, and the Gross-Pitaevskii equation is always valid.

In any real situation the total number of particles must of course be finite. Recalling that it is assumed that nearly all the particles are in the condensate mode $\psi(\mathbf{x})$, it is clear that once depletion starts to become significant, this approach can be problematical. In the systematic (and equivalent) expansions of C.W. Gardiner [10], and of Castin and Dum [11], there are in principle further terms which can be incorporated to account for higher order effects. Morgan [12] has taken a slightly different approach by only requiring that the occupation of the condensate mode be large, i.e. it may be significantly different from the total particle number, and adding in perturbative corrections to the Gross-Pitaevskii and Bogoliubov equations. This treatment, however, is designed for studying essentially steady-state BECs at finite temperature, rather than the explicitly dynamical sorts of situations described here.

The *theoretical* treatment of such situations is clearly a difficult problem, it is however likely relevant to coming generations of BEC experiments. If one actually wants to *do* something with a BEC, this will involve dynamics. As generic Gross-Pitaevskii equations are presumably non-integrable, there exists the definite possibility of chaos

and instability in some circumstances; this in turn implies the possibility of rapid depletion of the condensate mode, and concomitant loss of the desirable property of *coherence* of the macroscopic matter wave. Given this, it is equally desirable that such processes be better understood; this thus seems a suitable “quantum challenge” for the 21st century!

References

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[3] See also the contribution by G.V. Shlyapnikov.

[4] See also the contribution by M. Kuś.

[5] For simplicity a discrete decomposition has been assumed. This restriction is unlikely to be qualitatively important however.

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